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Study of magnetism and hybridization through ultrasonic attenuation in cuprate systems

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Abstract : In the present communication, an attempt is made to present a microscopic theoretical model for the cuprate systems in presence of antiferromagnetism (AFM), the position of impurity *f*-level, hybridization between *f*-level and copper *d*-electrons as well as phonon interaction to the hybridization in harmonic phonon vibration approximation When the high frequency ultrasonic wave travels in the solid, it deforms the lattice In our theoretical model calculation, the phonon Green's function is evaluated by Zubarev's technique The imaginary part of the phonon self-energy gives the ultrasonic attenuation of the system and displays the interplay of AFM and hybridization in it The effect of model parameters like staggered magnetic field (h), position of *f*-level (ϵ_f), hybridization (V), and electron-phonon coupling constant (g) on the temperature variation of ultrasonic attenuation is studied and the results are reported

Keywords : High-T_c cuprate superconductors, electron-phonon interaction

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1. Introduction

Ultrasonic methods are extremely valuable in elucidating the electron-phonon mechanism in strongly correlated electron systems. The ultrasonic peak and minimum in velocity are found in non-superconducting sample of NCCO at 260 K and in the superconducting sample at 200 K [1]. At low frequences and temperatures below 200 K, the attenuation increases with decreasing temperature and frequency and possibly arises due to interaction with the motion of domain wall. The attenuation arises possibly due to structural phase transition. A low tem-perature transformation from the orthorhombic to the tetragonal low temperature phase is observed with partial lattice stiffening and a small attenuation peak at $T < T_c$ is observed in LSCO [2]. Again attenuation measurements on LSCO showed two peaks, one close to the superconducting transition (T_c = 37.9 K) possibly combined with same structural instabilities and another at T_N = 27 K possibly of magnetic origin. Though some ultrasonic measurements are reported for NCCO and LSCO compounds, further experimental details are needed. The measurements do not show the effects of the hybridisation, antiferromagnetism. The

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microscopic theory of ultrasonic attenuation has not yet been reported. We propose a microscopic theoretical model to describe ultrasonic attenuation of high-T_c systems in normal phase in presence of antiferromagnetism (AFM), the position of *f*-level, hybridization between *f*-level and Cu *d*-electrons as well as phonon interaction to the hybridization in harmonic phonon vibration approximation. Behera and co-workers have investigated the velocity of sound [3] on this type of model. The under-doped systems exhibit AFM with low magnetic moments of the Cu^{2+} ion in CuO_2 plane. When the high frequency ultrasonic wave travels in the solid, it deforms the lattice and sets up lattice vibration. In our theoretical model calculation, the phonon Green's function is evaluated by Zubarev's technique [4].

2. Formalism

The Hamiltonian in *k*-space for the cuprate system is taken as

$$\mathcal{H}_o = \mathcal{H}_d + \mathcal{H}_s + \mathcal{H}_v + \mathcal{H}_f , \tag{1}$$

where

$$\mathcal{H}_d = \sum_{k,\sigma} \epsilon_0(k)\left(a^{\dagger}_{k,\sigma} b_{k,\sigma} + h.c.\right), \tag{2}$$

$$H_s = (h/2)\sum_{k,\sigma} \sigma\left(a^{\dagger}_{k,\sigma} a_{k,\sigma} - b^{\dagger}_{k,\sigma} b_{k,\sigma}\right), \tag{3}$$

$$\mathcal{H}_v = V\sum_{k,\sigma}\left(a^{\dagger}_{k,\sigma} f_{1,k,\sigma} + b^{\dagger}_{k,\sigma} f_{1,k,\sigma} + h.c.\right), \tag{4}$$

$$\mathcal{H}_f = \epsilon_f \sum_{k,\sigma} f^{\dagger}_{1,k,\sigma} f_{1,k,\sigma} . \tag{5}$$

$\mathcal{H}_d$, $\mathcal{H}_s$, $\mathcal{H}_v$ and $\mathcal{H}_f$ are conduction electron, staggered field, hybridization interaction and *f*-electron Hamiltonian, respectively. The Fourier transformed electron-phonon interaction Hamiltonian is

$$H_{e-p} = \sum_{k,q,\sigma} f(q)\left[\left(a^{\dagger}_{k+q,\sigma} f_{1,k,\sigma} + b^{\dagger}_{k+q,\sigma} f_{1,k,\sigma}\right) + h.c.\right] A_q \tag{6}$$

with $A_q = b_q + b^{\dagger}_{-q}$ where b_q ($b^{\dagger}_q$) are annihilation (creation) operators for phonon with wave vector q and $f(q)$ is the electron-phonon coupling constant. The free phonon Hamiltonian with phonon energy ω_q is written as $\mathcal{H}_p = \sum_q \omega_q b^{\dagger}_q b_q$. Hence the total Hamiltonian of the system is described by [3]

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{e-p} + \mathcal{H}_p . \tag{7}$$

3. Calculation of renormalized phonon energy

The double time phono Green's function of Zubarev [4] type is defined as

$$D_{q,q'}(t-t') = \ll A_q(t);\ A_{q'}(t') \gg$$
$$= -i\Theta(t-t') \left\langle \left[A_q(t); A_{q'}(t')\right] \right\rangle . \tag{8}$$

Applying Dyson approximation, the phonon Green's function can be written as

$$D_{q,q}(\omega) = (\omega_q / \pi)\left[\omega^2 - \omega_q^2 - \Sigma_q(\omega)\right]^{-1}, \tag{9}$$

where phonon self energy is given by

$$\sum_q(\omega) = 4\pi f^2(-q)\omega_q \chi_{qq}(\omega), \tag{10}$$

$$\chi_{q,q'}(\omega) = \sum_{k,k',\sigma,\sigma'}[\Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4]. \tag{11}$$

$\Gamma_i(k,k',q,q',\omega)$'s ($i = 1$ to 4) represent the electron response functions. We make some approximations, while calculating the electron response function, keeping the essential physics intact. We use certain decoupling schemes for the higher order Green's functions such that all the physical parameters like f-level, staggered magnetic field, hybridization term ($\sim V^2$) and phonon coupling term are retained. The limit of zero wave vector ($q \rightarrow 0$) and finite temperature are considered in evaluating the response function.

4. Expression for ultrasonic attenuation coefficient (α)

The high frequency ultrasonic sound wave, as it travels through the cuprate system, the lattice gets distorted giving rise to a new vibrational spectrum (phonon). The ultrasound is absorbed by the system corresponding to some appropriate energy of the sub-atomic system. This gives an idea about the electron configuration of the sub-atomic system. The ultrasonic attenuation coefficient $\alpha(\omega,T)$ for sound waves of frequency ω and at temperature T of the system is given by the imaginary part of the phonon self-energy. Mathematically it is written as

$$\alpha(\omega,T) = -\frac{2\pi}{\upsilon}\mathrm{Im}\,\chi(q=0,\omega), \tag{12}$$

where $\chi(q = 0,\omega)$ is the phonon response function for long wave length longitudinal phonons ($q \rightarrow 0$). The renormalised velocity of sound υ is given by

$$\upsilon = \sqrt{1+4A_2(\omega)}$$

and the ultrasonic attenuation co-efficient α is written as

$$\alpha = \frac{4B_2}{\sqrt{1+4A_2}}, \tag{13}$$

where the functional dependence of A_2 and B_2 on frequency and the model parameters has been calculated in detail. Different parameters used in the eq. (13) are made dimensionless by dividing them by hopping integral $2t_0$, where the width of the conduction band is $W = 8t_0$. Those are :

$$g = f^2(0)N(0)/\omega_0;\ d = \epsilon_f/2t_0;\ c = \omega/2t_0;$$

$$v = V/2t_0;\ e = \eta/2t_0;\ p = \omega_0/2t_0;\ \tilde{\omega} = c/p;$$

$$x_0 = \epsilon_0(k)/2t_0;\ \tilde{h} = h/2t_0;\ t = k_B T/2t_0;$$

where k_B is the Boltzmann constant.

5. Results and discussion

Figure 1 shows the temperature dependence of the attenuation when the electron-phonon coupling strength *(g)* varies representing different high-T_c superconducting compounds containing R-atoms When ultra sound interacts stongly with the electronic sub-system of the solid, it strongly modulates the *f*-electron and the conduction electron orbitals This causes the increase in hybridization (v) and hence increases the electron-phonon coupling strength *(g)* We investigate here the effect of the electron-phonon coupling on the attenuation co-efficient (α) It is observed from the Figure 1 that ultrasonic attenuation increases, as the electron-phonon coupling increases from g = 0 0180 to 0 0255 Attenuation peaks at temperature t = 0.10 corresponding to the fixed position of the *f*-level at d = 0 06 which is the middle of the hybridization gap.

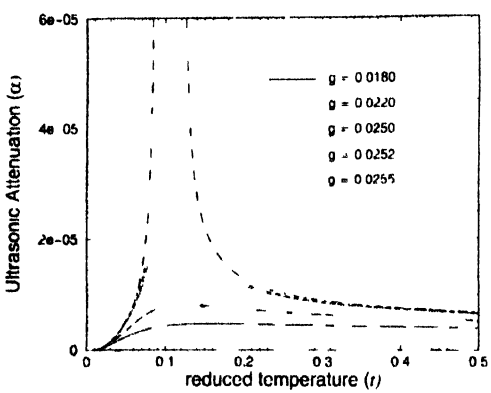

Figure 1. The plot of ultrasonic attenuation *vs* reduced temperature for fixed values of e = 0 018 p = 1 0, d = 0 06, v = 0 015, $h1$ = 0 195 t = 0 09, ω = 0 1 and for different values of g = 0 0180, 0 0220, 0 025, 0 0252, 0 0255

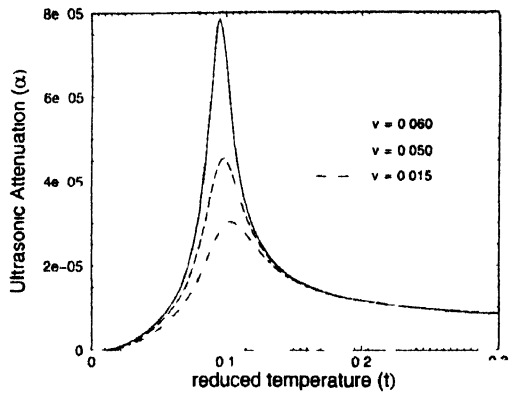

Figure 2 The plot of ultrasonic attenuation *vs* reduced temperature for fixed values of e = 0 018 p = 1 0, g = 0 025, d = 0 06, $h1$ = 0 195, ω = 0 1 and for different values of v = 0 07, 0 05, 0 015

Figure 2 shows the temperature dependence of the attenuation due to the hybridization (v) between the *f*-electrons and the conduction electrons. Though small, the high-T_c systems possess different magnitudes of hybridization strength. When ultrasonic sound interacts with the electrons, it deforms the lattice and enhances the hybridization This process causes damping of the ultrasonic wave and hence producing ultrasonic absorption It is worthwhile to mention here that the attenuation peak becomes sharper for stronger strength of the hybridization parameter

Figure 3 shows the temperature dependence of ultrasonic attenuation (α) for different ultrasonic frequencies The high frequency waves distort the lattice more, thereby increase the hybridization of the *f*-electrons and the conduction electrons. The attenuation increases with the increase of hybridization and also with increase in frequency (ω) and becomes sharper at higher frequencies. The attenuation decreases with decrease of temperature and becomes zero at temperature t = 0; but the

attenuation decreases more slowly and remains nearly constant at higher temperature.

In studying the temperature variation of ultrasonic attenuation for the system, from Figure 1 to Figure 3, we have considered a constant staggered magnetic field $h1$. But the staggered field varies with temperature. This temperature variation of $h1$ can be shown by a simple BCS type expression (Not shown here). Taking into account this type of temperature variation of $h1$, the temperature variation of 'α' is shown in Figure 4.

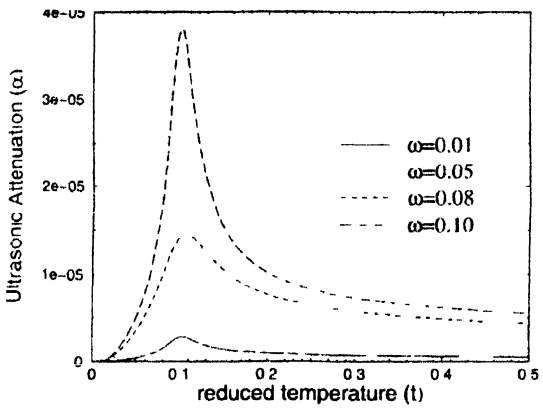

Figure 3. The plot of ultrasonic attenuation *vs.* reduced temperature for fixed values of $e = 0.018$, $p = 1.0$, $g = 0.025$, $d = 0.06$, $v = 0.015$, $h1 = 0.195$ and for different values of $\omega = 0.01, 0.05, 0.08, 0.10$.

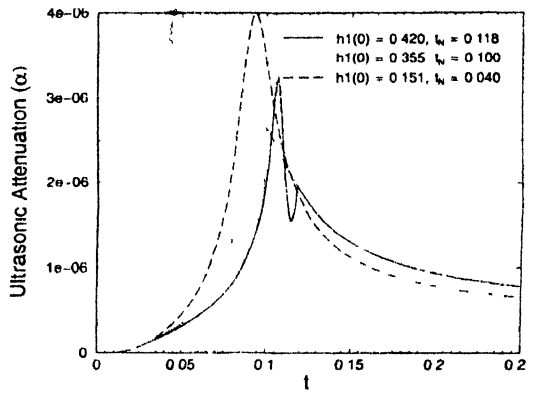

Figure 4. The plot of ultrasonic attenuation *vs.* reduced temperature for fixed values of the Néel temperature $t_N = 0.018, 0.100, 0.040$ with corresponding values of $h1(0)$ and $h1$ value as per BCS type variation *i.e.* $h1 = h1(0)h1 = h1(0)\left[1-(t/t_N)^2\right]^{1/2}$ and for fixed values of $e = 0.018$, $p = 1\ 0$, $g = 0\ 025$, $d = 0.06$, $v = 0.015$.

The Figure 4 shows the ultrasonic absorption peaks, one at Néel temperature t_N and another at hybridization gap at t^* with $t_N > t^*$. It is also observed that at $t_N < t^*$, only the absorption peak of staggered field gap appears but the hybridization gap disappears altogather. It is further noticed that ultrasonic peak shows asymmetry in its peak in magnetic phase for $t < t_N$. The ultrasonic absorption decreases rapidly in non-magnetic low-T phase, while absorption decreases more slowly for temperature $t > t_N$. This asymmetry in ultrasonic peak is a clear indication of the presence of two different phases in the system. Below the characteristic temperature t^* the hybridization effect is suppressed, so that the system containing localised *f*-level exhibits heavy fermion behaviour even in presence of antiferromagnetism. The weak hybridization between the lattice of 4*f*-ions of Nd with the strongly correlated electrons of Cu–O plane is observed experimentally [5].

The Figure 5 shows the effect of the position *f*-level *(d)* on the ultrasonic absorption peaks in which we observe two peaks. The high temperature peak is due to the ab-sorption of sound energy through the AFM gap, while the low temperature gap is due to absorption through hybridization gap. When *f*-level approaches the Fermi

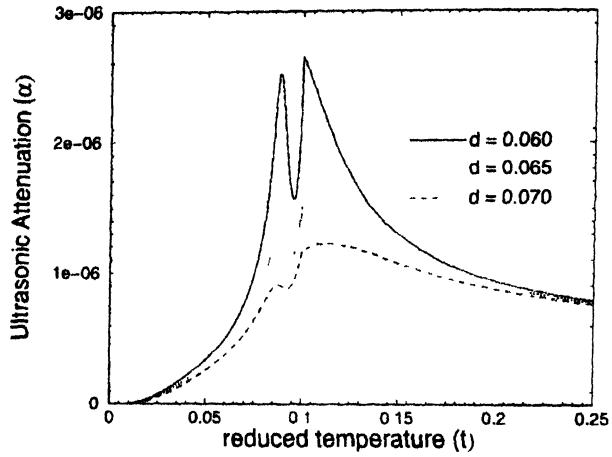

Figure 5. The plot of α *vs.* t for Néel temperature $t_N = 0.1$ with corresponding value of $h1(0) = 0.335$ and $h1$ value as per BCS type variation *i.e.* $h1 = h1(0)\left[1-(t/t_N)^2\right]^{1/2}$ and for fixed values of $e = 0.018$, $p = 1.0$, $g = 0.025$, $v = 0.15$, and with the different values of d.

level (from $d = 0.070$ to 0.060), the two peaks become sharp with decreasing line width of both the peaks. This happens because of the strong hybridization. When the *f*-level approaches the Fermi level, phonon coupling to the hybridization between the *f*- and *c*-electrons become stronger leading to increasing absorption of sound energy. In other words, when *f*-level moves away from the Fermi level, the hybridization becomes weaker and hence the two peaks become flat and ultimately merge to a single flat peak.

6. Conclusion

We calculated the temperature dependence of ultrasonic absorption coefficient (α) for the cuprate system in normal phase. The phonon coupling to the hybridization between *f*-electrons and conduction electrons is considered in the formalism of the model in presence of an anti-ferromagnetic (AFM) ground state. Introducing a simple BCS type temperature variation of the stagged field ($h1$). we observed two peaks in the α vs. t plot (Figure 5), one at $t_N \approx 0.118$ and shifted hybridization gap at $t^* \approx 0.107$ for a strong staggered field $h1(0) = 0.420$. Similar peaks at the staggered field is observed by Zhang *et al* [6] for the ultrasonic measurements in LSCO system.

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